

1,3-diphenyl-1,3-diazetidine
74949-76-1 | DTXSID60321268

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 809 L/kg

Global applicability domain: Outside

Local applicability domain index: 3.34e-01

Confidence level: 5.38e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4,4'-Methylenebis(N,N-dimethylaniline)</div> <div>Measured: 9120</div> <div>Predicted: 3540</div>	<div>Image not found</div> <div>Auramine</div> <div>Measured: 2040</div> <div>Predicted: 1020</div>	<div>Image not found</div> <div>Michler's ketone</div> <div>Measured: 162</div> <div>Predicted: 489</div>
<div>Image not found</div> <div>Methapyrilene</div> <div>Measured: 741</div> <div>Predicted: 682</div>	<div>Image not found</div> <div>Hexazinone</div> <div>Measured: 53.7</div> <div>Predicted: 67.1</div>	